



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:05 PM GMT

PDB ID : 1WEK  
Title : Crystal structure of the conserved hypothetical protein TT1465 from *Thermus thermophilus* HB8  
Authors : Kukimoto-Niino, M.; Murayama, K.; Kato-Murayama, M.; Terada, T.; Shirouzu, M.; Kuramitsu, S.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2004-05-25  
Resolution : 2.20 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.

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The following versions of software and data (see [references ⓘ](#)) 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

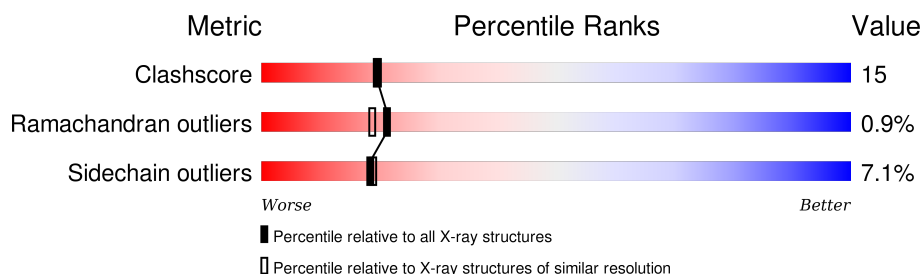
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	217	
1	B	217	
1	C	217	
1	D	217	
1	E	217	
1	F	217	

## 2 Entry composition [i](#)

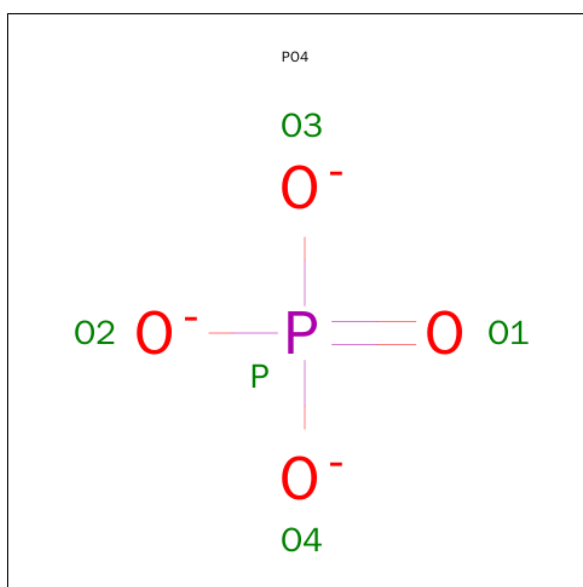
There are 3 unique types of molecules in this entry. The entry contains 10248 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 hypothetical protein TT1465.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	Se	0	0	0
			1651	1076	281	293	1			
1	B	207	Total	C	N	O	Se	0	0	0
			1644	1071	280	292	1			
1	C	206	Total	C	N	O	Se	0	0	0
			1632	1066	277	288	1			
1	D	208	Total	C	N	O	Se	0	0	0
			1646	1074	279	292	1			
1	E	206	Total	C	N	O	Se	0	0	0
			1629	1062	276	290	1			
1	F	205	Total	C	N	O	Se	0	0	0
			1624	1060	276	287	1			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0

- Molecule 3 is water.

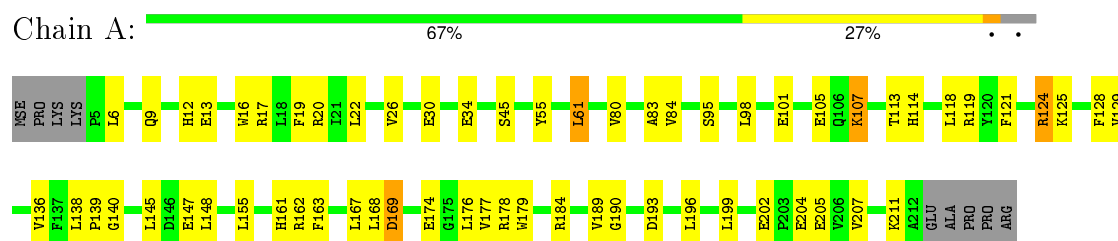
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	75	Total O 75 75	0	0
3	B	56	Total O 56 56	0	0
3	C	48	Total O 48 48	0	0
3	D	51	Total O 51 51	0	0
3	E	65	Total O 65 65	0	0
3	F	67	Total O 67 67	0	0

### 3 Residue-property plots

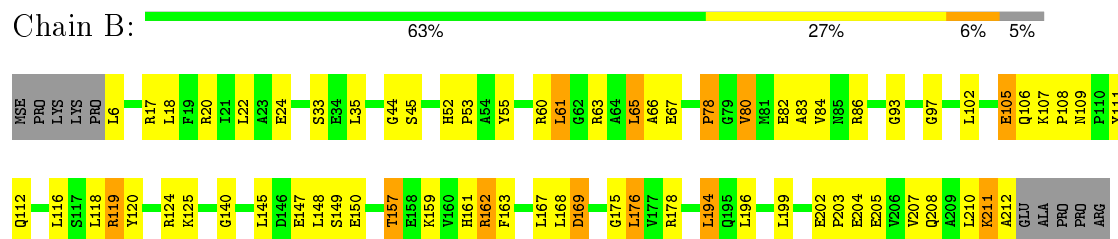
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

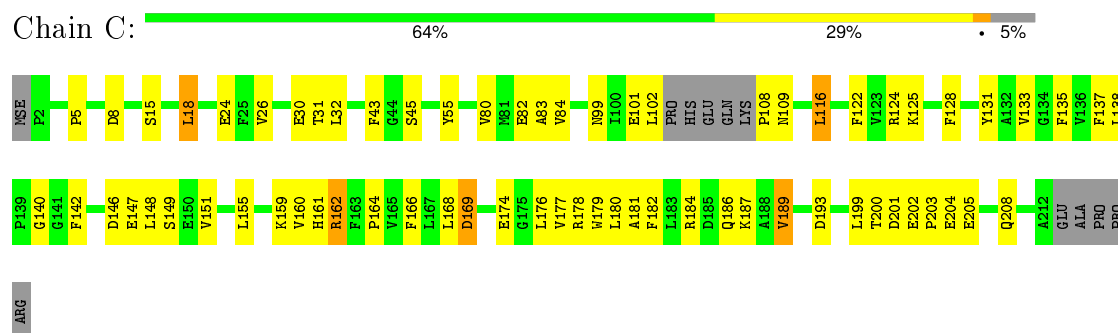
- Molecule 1: hypothetical protein TT1465



- Molecule 1: hypothetical protein TT1465

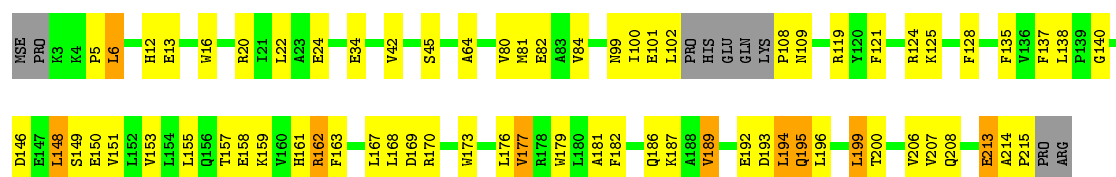


- Molecule 1: hypothetical protein TT1465



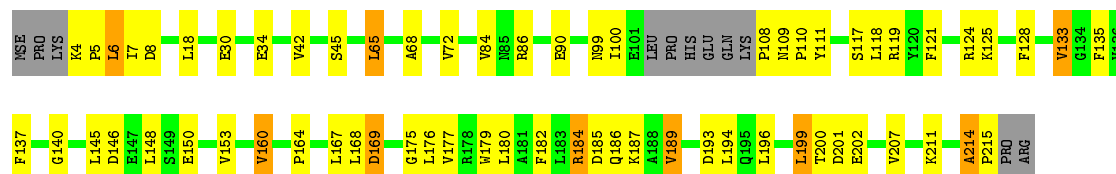
- Molecule 1: hypothetical protein TT1465





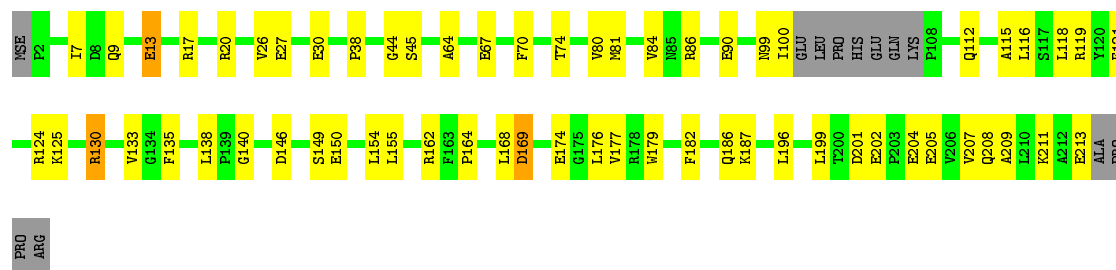
- Molecule 1: hypothetical protein TT1465

Chain E: 65% 26% 5%



- Molecule 1: hypothetical protein TT1465

Chain F: 66% 27% 6%



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.65Å 83.80Å 265.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.94 – 2.20	Depositor
% Data completeness (in resolution range)	93.9 (14.94-2.20)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.198 , 0.250	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10248	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

## 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: PO4

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	0/1695	0.63	0/2298
1	B	0.43	0/1687	0.64	0/2287
1	C	0.41	0/1674	0.62	0/2266
1	D	0.40	0/1688	0.60	0/2286
1	E	0.43	0/1671	0.63	0/2264
1	F	0.44	0/1666	0.61	0/2255
All	All	0.42	0/10081	0.62	0/13656

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 [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	1651	0	1627	60	0
1	B	1644	0	1619	56	0
1	C	1632	0	1619	52	0
1	D	1646	0	1629	56	0
1	E	1629	0	1605	50	0
1	F	1624	0	1608	51	0
2	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	0	0
2	C	15	0	0	1	0
2	D	15	0	0	1	0
2	E	10	0	0	0	0
2	F	10	0	0	0	0
3	A	75	0	0	3	0
3	B	56	0	0	3	0
3	C	48	0	0	3	0
3	D	51	0	0	1	0
3	E	65	0	0	1	0
3	F	67	0	0	4	0
All	All	10248	0	9707	291	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 15.

All (291) 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:C:200:THR:HG22	1:C:202:GLU:H	1.24	1.03
1:D:81:MSE:HE2	1:D:81:MSE:HA	1.52	0.88
1:F:202:GLU:HB2	1:F:205:GLU:HG3	1.55	0.87
1:A:107:LYS:HD2	1:A:107:LYS:H	1.37	0.86
1:C:159:LYS:NZ	1:D:102:LEU:HD23	1.95	0.81
1:E:30:GLU:O	1:E:34:GLU:HG2	1.81	0.81
1:F:13:GLU:HB2	3:F:519:HOH:O	1.79	0.81
1:D:157:THR:HG21	1:D:159:LYS:NZ	1.96	0.80
1:E:184:ARG:HG3	1:E:185:ASP:N	1.96	0.80
1:B:157:THR:HG23	1:B:159:LYS:HG2	1.63	0.80
1:B:61:LEU:HD22	1:B:65:LEU:HD22	1.64	0.79
1:D:151:VAL:O	1:D:155:LEU:HD23	1.82	0.79
1:B:178:ARG:HG2	1:B:178:ARG:HH11	1.48	0.78
1:A:167:LEU:HB2	1:A:199:LEU:HD13	1.63	0.78
1:E:7:ILE:HG22	1:F:130:ARG:HG2	1.67	0.77
1:C:159:LYS:HZ1	1:D:102:LEU:HD23	1.49	0.77
1:C:45:SER:HB2	1:C:140:GLY:HA2	1.66	0.76
1:A:145:LEU:CD1	1:B:149:SER:HB3	2.15	0.76
1:F:45:SER:HB2	1:F:140:GLY:HA2	1.66	0.76
1:B:204:GLU:O	1:B:208:GLN:HG2	1.86	0.75
1:F:45:SER:O	1:F:80:VAL:HG12	1.86	0.75
1:A:155:LEU:HD22	1:A:162:ARG:HA	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:99:ASN:HD21	1:F:112:GLN:HE22	1.36	0.73
1:A:107:LYS:HD2	1:A:107:LYS:N	2.04	0.73
1:D:157:THR:HG21	1:D:159:LYS:HZ3	1.53	0.72
1:E:7:ILE:HD11	1:E:121:PHE:HE2	1.53	0.72
1:C:202:GLU:HG3	1:C:205:GLU:HG3	1.71	0.72
1:E:68:ALA:HB1	1:E:211:LYS:HD3	1.69	0.72
1:D:45:SER:HB2	1:D:140:GLY:HA2	1.71	0.71
1:A:167:LEU:HB2	1:A:199:LEU:CD1	2.20	0.70
1:C:204:GLU:HG3	1:C:208:GLN:HE21	1.55	0.70
1:A:45:SER:HB2	1:A:140:GLY:HA2	1.74	0.69
1:C:101:GLU:C	1:C:102:LEU:HD12	2.13	0.68
1:E:200:THR:HG22	1:E:201:ASP:N	2.07	0.68
1:C:122:PHE:HA	1:C:125:LYS:HD3	1.76	0.68
1:D:99:ASN:ND2	1:D:108:PRO:HB3	2.10	0.67
1:B:44:GLY:HA3	1:B:80:VAL:CG2	2.25	0.67
1:E:42:VAL:HG11	1:E:84:VAL:HG21	1.77	0.67
1:A:113:THR:HG22	1:A:114:HIS:CD2	2.30	0.66
1:D:42:VAL:HG11	1:D:84:VAL:HG21	1.77	0.66
1:C:149:SER:HB3	1:D:146:ASP:HA	1.78	0.66
2:C:507:PO4:O3	1:D:12:HIS:HD2	1.79	0.66
1:B:162:ARG:HD2	3:B:512:HOH:O	1.94	0.66
1:E:45:SER:HB2	1:E:140:GLY:HA2	1.78	0.65
1:E:167:LEU:HB2	1:E:199:LEU:HD22	1.79	0.65
1:C:204:GLU:O	1:C:208:GLN:HG2	1.95	0.65
1:C:138:LEU:HD21	1:C:168:LEU:HD12	1.78	0.64
1:E:99:ASN:ND2	1:E:108:PRO:HB3	2.13	0.64
1:C:26:VAL:O	1:C:30:GLU:HG3	1.96	0.64
1:A:161:HIS:HB3	1:A:163:PHE:CE1	2.31	0.64
1:A:98:LEU:O	1:A:124:ARG:HD2	1.97	0.64
1:E:65:LEU:HD13	1:E:207:VAL:HG22	1.79	0.64
1:A:155:LEU:CD2	1:A:162:ARG:HA	2.28	0.63
1:B:161:HIS:ND1	1:B:162:ARG:O	2.30	0.63
1:D:81:MSE:CE	1:D:81:MSE:HA	2.27	0.63
1:B:157:THR:CG2	1:B:159:LYS:HG2	2.27	0.63
1:E:146:ASP:HA	1:F:149:SER:HB3	1.81	0.62
1:D:157:THR:HG22	1:D:159:LYS:HG3	1.82	0.62
1:D:20:ARG:O	1:D:24:GLU:HG3	2.01	0.61
1:A:12:HIS:ND1	1:B:33:SER:HB2	2.15	0.61
1:E:200:THR:HG22	1:E:202:GLU:H	1.65	0.61
1:F:7:ILE:HD11	1:F:121:PHE:HZ	1.66	0.61
1:F:162:ARG:HG3	1:F:162:ARG:HH11	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:LYS:H	1:A:107:LYS:CD	2.13	0.60
1:A:145:LEU:CD1	1:B:149:SER:CB	2.80	0.60
1:E:189:VAL:HG13	1:E:193:ASP:HB2	1.84	0.60
1:D:162:ARG:HD3	1:D:162:ARG:O	2.02	0.60
1:A:61:LEU:HD11	1:A:136:VAL:HG11	1.82	0.59
1:A:177:VAL:HG21	1:A:199:LEU:HD22	1.84	0.59
1:E:200:THR:HG22	1:E:201:ASP:H	1.65	0.59
1:C:82:GLU:HG3	1:C:109:ASN:HB2	1.85	0.59
1:E:7:ILE:CG2	1:F:130:ARG:HG2	2.33	0.59
1:B:202:GLU:HB3	1:B:205:GLU:HG3	1.85	0.59
1:D:125:LYS:HD2	1:D:150:GLU:HG3	1.84	0.59
1:A:125:LYS:HD3	1:A:147:GLU:OE1	2.02	0.59
1:C:189:VAL:HG13	1:C:193:ASP:HB2	1.85	0.59
1:E:125:LYS:HD3	1:E:150:GLU:OE1	2.04	0.58
1:F:74:THR:HB	1:F:81:MSE:HG3	1.84	0.58
1:A:202:GLU:HB3	1:A:204:GLU:CD	2.23	0.58
1:A:22:LEU:HD11	1:B:22:LEU:HD21	1.84	0.58
1:C:137:PHE:HE2	1:C:147:GLU:HB3	1.69	0.57
1:F:81:MSE:SE	3:F:553:HOH:O	2.71	0.57
1:C:18:LEU:HD23	1:D:22:LEU:HD22	1.86	0.57
1:D:189:VAL:HG13	1:D:193:ASP:HB2	1.87	0.57
1:F:125:LYS:HD3	1:F:150:GLU:OE1	2.05	0.57
1:F:7:ILE:HD11	1:F:121:PHE:CZ	2.39	0.57
1:E:160:VAL:HG13	1:F:7:ILE:HD12	1.87	0.56
1:B:63:ARG:O	1:B:67:GLU:HG3	2.04	0.56
1:C:181:ALA:O	1:C:184:ARG:HG2	2.04	0.56
1:E:86:ARG:O	1:E:90:GLU:HG3	2.05	0.56
1:B:44:GLY:HA3	1:B:80:VAL:HG21	1.86	0.56
1:F:207:VAL:HG12	1:F:211:LYS:HD2	1.88	0.56
1:C:80:VAL:O	1:C:84:VAL:HG23	2.06	0.56
1:B:44:GLY:HA3	1:B:80:VAL:HG22	1.88	0.56
1:D:173:TRP:O	1:D:177:VAL:HG13	2.05	0.56
1:E:179:TRP:O	1:E:182:PHE:HB3	2.05	0.56
1:F:100:ILE:HG12	1:F:124:ARG:NH1	2.21	0.56
1:D:137:PHE:HB2	1:D:167:LEU:HD23	1.87	0.56
1:D:155:LEU:HD21	1:D:163:PHE:CZ	2.41	0.55
1:A:6:LEU:H	1:A:6:LEU:HD23	1.71	0.55
1:E:117:SER:C	1:E:118:LEU:HD12	2.27	0.55
1:C:138:LEU:HD23	1:C:168:LEU:HB2	1.89	0.55
1:B:161:HIS:ND1	1:B:162:ARG:N	2.55	0.55
1:C:176:LEU:O	1:C:180:LEU:HG	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:ARG:NH1	1:B:178:ARG:HG2	2.17	0.55
1:B:80:VAL:O	1:B:84:VAL:HG23	2.07	0.55
1:E:7:ILE:HD11	1:E:121:PHE:CE2	2.38	0.54
1:D:213:GLU:HG2	1:D:214:ALA:N	2.21	0.54
1:D:192:GLU:O	1:D:195:GLN:HB2	2.06	0.54
1:A:26:VAL:O	1:A:30:GLU:HG3	2.06	0.54
1:D:157:THR:HG21	1:D:159:LYS:HZ2	1.72	0.54
1:C:182:PHE:CE1	1:C:186:GLN:NE2	2.75	0.54
1:D:179:TRP:O	1:D:182:PHE:HB3	2.07	0.54
1:B:202:GLU:HG3	1:B:204:GLU:OE1	2.09	0.53
1:B:211:LYS:O	1:B:211:LYS:HG2	2.08	0.53
1:F:177:VAL:HG21	1:F:199:LEU:HD11	1.90	0.53
1:A:121:PHE:HE1	1:B:159:LYS:HG3	1.73	0.53
1:B:161:HIS:HD1	1:B:162:ARG:N	2.07	0.53
1:A:80:VAL:O	1:A:84:VAL:HG23	2.09	0.52
1:B:167:LEU:HB2	1:B:199:LEU:HD13	1.90	0.52
1:E:109:ASN:HD22	1:E:111:TYR:H	1.57	0.52
1:C:55:TYR:CD1	1:C:83:ALA:HB2	2.44	0.52
1:D:153:VAL:O	1:D:157:THR:HB	2.09	0.52
1:A:121:PHE:CE1	1:B:159:LYS:HG3	2.45	0.52
1:C:116:LEU:N	1:C:116:LEU:HD23	2.24	0.52
1:D:186:GLN:O	1:D:187:LYS:HB2	2.09	0.52
1:D:100:ILE:HD11	1:D:124:ARG:HD2	1.90	0.52
1:A:101:GLU:OE2	1:A:119:ARG:HG2	2.09	0.52
1:A:95:SER:H	1:A:113:THR:HB	1.75	0.52
1:F:38:PRO:HB2	1:F:70:PHE:HD2	1.74	0.52
1:B:162:ARG:HG3	1:B:163:PHE:N	2.25	0.52
1:A:184:ARG:HA	1:A:189:VAL:HG12	1.91	0.52
1:D:176:LEU:HD13	1:D:176:LEU:C	2.30	0.52
1:F:9:GLN:HE22	1:F:119:ARG:HH22	1.57	0.51
1:B:168:LEU:O	1:B:169:ASP:HB3	2.11	0.51
1:C:177:VAL:HG21	1:C:199:LEU:HD21	1.92	0.51
1:B:45:SER:HB2	1:B:140:GLY:HA2	1.92	0.51
1:E:200:THR:CG2	1:E:201:ASP:N	2.74	0.51
1:A:207:VAL:O	1:A:211:LYS:HG3	2.11	0.51
1:B:78:PRO:HG2	1:B:106:GLN:HG2	1.93	0.51
1:C:164:PRO:HB2	1:C:166:PHE:CE1	2.46	0.51
1:F:179:TRP:O	1:F:182:PHE:HB3	2.11	0.50
1:B:204:GLU:CD	1:B:204:GLU:H	2.14	0.50
1:F:162:ARG:HG3	1:F:162:ARG:NH1	2.26	0.50
1:C:184:ARG:HB2	3:C:550:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ARG:NH2	1:F:27:GLU:HG2	2.26	0.50
1:C:147:GLU:O	1:C:151:VAL:HG23	2.11	0.50
1:F:38:PRO:HB2	1:F:70:PHE:CD2	2.46	0.50
1:B:86:ARG:HD2	1:B:111:TYR:CE1	2.46	0.50
1:E:4:LYS:HE3	1:E:8:ASP:HB3	1.93	0.50
1:A:161:HIS:HD2	1:A:163:PHE:CE2	2.30	0.50
1:F:119:ARG:NH1	3:F:511:HOH:O	2.44	0.50
1:C:149:SER:CB	1:D:146:ASP:HA	2.42	0.49
1:D:157:THR:CG2	1:D:157:THR:O	2.60	0.49
1:C:179:TRP:O	1:C:182:PHE:HB3	2.12	0.49
1:F:86:ARG:O	1:F:90:GLU:HG3	2.12	0.49
1:D:16:TRP:CZ3	1:F:13:GLU:HG3	2.47	0.49
1:F:64:ALA:HB1	1:F:207:VAL:HG21	1.94	0.49
1:E:153:VAL:HG21	1:F:146:ASP:HB2	1.94	0.49
1:B:97:GLY:HA3	1:B:112:GLN:NE2	2.28	0.49
1:D:101:GLU:OE1	1:D:119:ARG:NE	2.45	0.49
1:B:210:LEU:C	1:B:212:ALA:H	2.15	0.49
1:D:6:LEU:HD11	1:D:119:ARG:O	2.13	0.49
1:E:214:ALA:H	1:E:215:PRO:CD	2.26	0.49
1:B:52:HIS:ND1	1:B:53:PRO:HD2	2.28	0.49
1:A:80:VAL:CG1	1:A:138:LEU:HD13	2.43	0.48
1:E:200:THR:CG2	1:E:201:ASP:H	2.27	0.48
1:A:179:TRP:CD1	1:B:175:GLY:HA3	2.48	0.48
1:C:15:SER:O	1:C:18:LEU:HB2	2.12	0.48
1:C:142:PHE:CE2	1:D:189:VAL:HG21	2.49	0.48
1:C:146:ASP:HA	1:D:149:SER:HB3	1.96	0.48
1:A:189:VAL:HG22	1:A:193:ASP:HB2	1.96	0.47
1:E:168:LEU:O	1:E:169:ASP:CB	2.62	0.47
1:A:189:VAL:HG22	1:A:193:ASP:OD2	2.14	0.47
1:E:133:VAL:O	1:E:164:PRO:HD2	2.13	0.47
2:D:512:PO4:O4	1:E:30:GLU:OE1	2.32	0.47
1:C:200:THR:HG23	1:C:205:GLU:OE1	2.13	0.47
1:A:105:GLU:HA	1:A:105:GLU:OE1	2.14	0.47
1:C:43:PHE:CD1	1:C:147:GLU:HG3	2.50	0.47
1:A:204:GLU:HG2	1:A:205:GLU:N	2.30	0.47
1:A:179:TRP:CZ3	1:B:176:LEU:HG	2.50	0.47
1:A:95:SER:O	1:A:113:THR:N	2.47	0.46
1:F:125:LYS:HD3	1:F:150:GLU:CD	2.35	0.46
1:A:9:GLN:O	1:A:13:GLU:HG3	2.16	0.46
1:F:186:GLN:O	1:F:187:LYS:HB2	2.15	0.46
1:F:44:GLY:HA3	1:F:80:VAL:HG11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:GLN:O	1:C:187:LYS:HB2	2.15	0.46
1:F:26:VAL:O	1:F:30:GLU:HG3	2.16	0.46
1:C:18:LEU:HD23	1:D:22:LEU:CD2	2.46	0.46
1:F:169:ASP:HA	1:F:201:ASP:OD1	2.16	0.46
1:B:20:ARG:O	1:B:24:GLU:HG3	2.16	0.46
1:F:80:VAL:O	1:F:84:VAL:HG23	2.15	0.46
1:B:60:ARG:HD2	3:B:547:HOH:O	2.16	0.46
1:F:9:GLN:NE2	1:F:119:ARG:HH22	2.14	0.45
1:E:200:THR:HG22	1:E:202:GLU:N	2.32	0.45
1:B:18:LEU:O	1:B:22:LEU:HB2	2.16	0.45
1:A:145:LEU:HD12	1:B:149:SER:CB	2.46	0.45
1:A:22:LEU:HD11	1:B:22:LEU:CD2	2.46	0.45
1:B:65:LEU:HD13	1:B:207:VAL:HG22	1.97	0.45
1:E:125:LYS:HD3	1:E:150:GLU:CD	2.36	0.45
1:F:202:GLU:CB	1:F:205:GLU:HG3	2.38	0.45
1:C:200:THR:HG22	1:C:201:ASP:N	2.32	0.44
1:C:31:THR:HG21	1:C:116:LEU:CD2	2.47	0.44
1:A:168:LEU:O	1:A:169:ASP:HB3	2.16	0.44
1:D:157:THR:O	1:D:158:GLU:HB2	2.18	0.44
1:C:174:GLU:HG2	1:C:178:ARG:NH2	2.33	0.44
1:A:129:VAL:HG23	3:A:563:HOH:O	2.17	0.44
1:D:80:VAL:CG1	1:D:138:LEU:HD13	2.47	0.44
1:C:102:LEU:HD12	1:C:102:LEU:N	2.31	0.44
1:E:65:LEU:HD23	1:E:72:VAL:HG12	2.00	0.44
1:B:86:ARG:HB2	1:B:111:TYR:CD1	2.53	0.44
1:C:174:GLU:HG2	1:C:178:ARG:HH22	1.83	0.44
1:B:119:ARG:HG2	1:B:120:TYR:CE1	2.52	0.44
1:C:168:LEU:O	1:C:169:ASP:CB	2.66	0.44
1:A:20:ARG:HB3	3:A:520:HOH:O	2.18	0.44
1:E:137:PHE:CZ	1:E:148:LEU:HA	2.53	0.44
1:B:125:LYS:HG2	1:B:147:GLU:OE2	2.18	0.44
1:F:204:GLU:O	1:F:208:GLN:HG3	2.17	0.44
1:E:153:VAL:HG21	1:F:146:ASP:CB	2.48	0.43
1:F:162:ARG:NH2	3:F:529:HOH:O	2.51	0.43
1:E:175:GLY:HA3	1:F:179:TRP:CD1	2.53	0.43
1:E:176:LEU:O	1:E:180:LEU:HG	2.18	0.43
1:D:5:PRO:HA	3:D:519:HOH:O	2.17	0.43
1:E:160:VAL:HG13	1:F:7:ILE:CD1	2.48	0.43
1:A:101:GLU:HG3	1:A:118:LEU:O	2.18	0.43
1:B:55:TYR:CE1	1:B:83:ALA:HB2	2.53	0.43
1:E:177:VAL:HG21	1:E:199:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:ARG:NH1	1:C:162:ARG:HG3	2.34	0.43
1:D:168:LEU:HA	1:D:200:THR:O	2.19	0.43
1:B:82:GLU:HG3	1:B:109:ASN:HB2	2.01	0.43
1:E:186:GLN:O	1:E:187:LYS:HB2	2.19	0.43
1:A:20:ARG:NH1	1:A:119:ARG:HG3	2.34	0.43
1:A:55:TYR:CE1	1:A:83:ALA:HB2	2.53	0.43
1:D:12:HIS:CE1	1:D:13:GLU:HG3	2.54	0.43
1:A:20:ARG:HD2	3:A:520:HOH:O	2.17	0.43
1:D:121:PHE:O	1:D:125:LYS:HG2	2.19	0.42
3:E:554:HOH:O	1:F:125:LYS:HD2	2.19	0.42
1:F:17:ARG:NH1	1:F:20:ARG:HH21	2.17	0.42
1:C:202:GLU:HA	1:C:203:PRO:HD3	1.87	0.42
1:F:164:PRO:HG2	1:F:213:GLU:OE1	2.19	0.42
1:B:211:LYS:HE2	1:B:211:LYS:HB3	1.86	0.42
1:F:168:LEU:O	1:F:169:ASP:CB	2.67	0.42
1:A:145:LEU:HD12	1:B:149:SER:HB3	1.97	0.42
1:E:109:ASN:HA	1:E:110:PRO:HD3	1.84	0.42
1:F:208:GLN:HE21	1:F:208:GLN:HB3	1.63	0.42
1:F:209:ALA:O	1:F:213:GLU:HG3	2.19	0.42
1:C:8:ASP:OD2	1:D:161:HIS:ND1	2.48	0.42
1:D:82:GLU:HG3	1:D:109:ASN:HB2	2.01	0.42
1:B:63:ARG:NH1	3:B:545:HOH:O	2.52	0.42
1:C:162:ARG:HG3	1:C:162:ARG:HH11	1.83	0.42
1:C:160:VAL:HG22	1:C:161:HIS:N	2.35	0.42
1:B:107:LYS:HA	1:B:108:PRO:HD3	1.85	0.42
1:C:168:LEU:O	1:C:169:ASP:HB3	2.19	0.42
3:C:513:HOH:O	1:D:150:GLU:HG2	2.19	0.42
1:A:190:GLY:N	1:A:193:ASP:OD2	2.50	0.42
1:A:174:GLU:HG3	1:A:178:ARG:HE	1.85	0.42
1:F:112:GLN:NE2	1:F:115:ALA:HA	2.34	0.42
1:A:174:GLU:O	1:A:178:ARG:HG3	2.19	0.42
1:A:19:PHE:CE2	1:E:18:LEU:HD12	2.54	0.42
1:E:6:LEU:HD11	1:E:119:ARG:O	2.20	0.42
1:B:194:LEU:HA	1:B:194:LEU:HD12	1.85	0.42
1:B:102:LEU:O	1:B:105:GLU:HG2	2.20	0.41
1:A:30:GLU:O	1:A:34:GLU:HG3	2.19	0.41
1:B:116:LEU:N	1:B:116:LEU:HD12	2.35	0.41
1:A:189:VAL:HG22	1:A:193:ASP:CB	2.51	0.41
1:E:4:LYS:HA	1:E:5:PRO:HD3	1.87	0.41
1:D:168:LEU:HD11	1:D:206:VAL:HG21	2.03	0.41
1:C:168:LEU:HA	1:C:200:THR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:PRO:HB3	1:D:158:GLU:O	2.20	0.41
1:D:34:GLU:OE2	1:E:119:ARG:NH2	2.45	0.41
1:D:170:ARG:HG2	1:D:199:LEU:HB3	2.02	0.41
1:C:99:ASN:ND2	1:C:108:PRO:HB3	2.35	0.41
1:D:214:ALA:HA	1:D:215:PRO:HD3	1.82	0.41
1:D:64:ALA:HB1	1:D:207:VAL:HG21	2.02	0.41
1:D:20:ARG:HD3	1:E:30:GLU:OE2	2.20	0.41
1:F:125:LYS:HD3	1:F:150:GLU:OE2	2.20	0.41
1:A:80:VAL:HG11	1:A:138:LEU:HD13	2.03	0.41
1:B:66:ALA:HB1	1:B:93:GLY:HA3	2.03	0.41
1:E:100:ILE:HB	1:E:124:ARG:NH2	2.36	0.41
1:D:148:LEU:HD12	1:D:173:TRP:CZ3	2.56	0.40
1:A:107:LYS:CD	1:A:107:LYS:N	2.74	0.40
1:C:32:LEU:HB3	1:C:131:TYR:CD1	2.57	0.40
1:A:55:TYR:CD1	1:A:83:ALA:HB2	2.57	0.40
1:B:202:GLU:HA	1:B:203:PRO:HD3	2.01	0.40
1:E:65:LEU:CD1	1:E:207:VAL:HG22	2.50	0.40
1:E:168:LEU:O	1:E:169:ASP:HB3	2.22	0.40
1:D:181:ALA:HA	1:D:194:LEU:HD21	2.03	0.40
1:F:155:LEU:HD22	1:F:162:ARG:HD3	2.04	0.40
3:C:513:HOH:O	1:D:125:LYS:NZ	2.55	0.40
1:A:138:LEU:O	1:A:139:PRO:C	2.57	0.40
1:A:16:TRP:CH2	1:A:17:ARG:CZ	3.04	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	206/217 (95%)	197 (96%)	8 (4%)	1 (0%)	34 35
1	B	205/217 (94%)	194 (95%)	7 (3%)	4 (2%)	9 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	202/217 (93%)	196 (97%)	5 (2%)	1 (0%)	34	35
1	D	204/217 (94%)	194 (95%)	9 (4%)	1 (0%)	34	35
1	E	202/217 (93%)	196 (97%)	4 (2%)	2 (1%)	19	16
1	F	201/217 (93%)	194 (96%)	5 (2%)	2 (1%)	19	16
All	All	1220/1302 (94%)	1171 (96%)	38 (3%)	11 (1%)	21	19

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	105	GLU
1	C	169	ASP
1	E	169	ASP
1	E	214	ALA
1	F	169	ASP
1	A	169	ASP
1	B	211	LYS
1	F	174	GLU
1	B	169	ASP
1	D	169	ASP
1	B	78	PRO

### 5.3.2 Protein sidechains ⓘ

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	169/175 (97%)	162 (96%)	7 (4%)	37	45
1	B	168/175 (96%)	151 (90%)	17 (10%)	9	8
1	C	167/175 (95%)	156 (93%)	11 (7%)	21	22
1	D	168/175 (96%)	155 (92%)	13 (8%)	16	16
1	E	166/175 (95%)	154 (93%)	12 (7%)	18	18
1	F	166/175 (95%)	155 (93%)	11 (7%)	21	22
All	All	1004/1050 (96%)	933 (93%)	71 (7%)	18	19

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	LEU
1	A	107	LYS
1	A	124	ARG
1	A	128	PHE
1	A	148	LEU
1	A	176	LEU
1	A	196	LEU
1	B	6	LEU
1	B	17	ARG
1	B	35	LEU
1	B	61	LEU
1	B	65	LEU
1	B	80	VAL
1	B	118	LEU
1	B	119	ARG
1	B	124	ARG
1	B	145	LEU
1	B	148	LEU
1	B	150	GLU
1	B	157	THR
1	B	162	ARG
1	B	176	LEU
1	B	194	LEU
1	B	196	LEU
1	C	18	LEU
1	C	24	GLU
1	C	116	LEU
1	C	124	ARG
1	C	128	PHE
1	C	133	VAL
1	C	135	PHE
1	C	148	LEU
1	C	155	LEU
1	C	162	ARG
1	C	189	VAL
1	D	6	LEU
1	D	128	PHE
1	D	135	PHE
1	D	148	LEU
1	D	162	ARG
1	D	177	VAL
1	D	189	VAL

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Mol	Chain	Res	Type
1	D	194	LEU
1	D	195	GLN
1	D	196	LEU
1	D	199	LEU
1	D	208	GLN
1	D	213	GLU
1	E	6	LEU
1	E	65	LEU
1	E	128	PHE
1	E	133	VAL
1	E	135	PHE
1	E	145	LEU
1	E	160	VAL
1	E	184	ARG
1	E	189	VAL
1	E	194	LEU
1	E	196	LEU
1	E	199	LEU
1	F	13	GLU
1	F	67	GLU
1	F	116	LEU
1	F	118	LEU
1	F	130	ARG
1	F	133	VAL
1	F	135	PHE
1	F	138	LEU
1	F	154	LEU
1	F	176	LEU
1	F	196	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	99	ASN
1	A	112	GLN
1	A	114	HIS
1	A	161	HIS
1	A	186	GLN
1	B	99	ASN
1	B	112	GLN
1	C	9	GLN
1	C	99	ASN

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Mol	Chain	Res	Type
1	C	112	GLN
1	C	195	GLN
1	C	208	GLN
1	D	12	HIS
1	D	52	HIS
1	D	99	ASN
1	D	112	GLN
1	D	114	HIS
1	D	195	GLN
1	E	36	GLN
1	E	99	ASN
1	E	109	ASN
1	E	112	GLN
1	E	114	HIS
1	E	186	GLN
1	F	9	GLN
1	F	85	ASN
1	F	112	GLN
1	F	208	GLN

### 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 ⓘ

12 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	PO4	A	501	-	4,4,4	1.09	0	6,6,6	0.27	0
2	PO4	B	503	-	4,4,4	1.02	0	6,6,6	0.27	0
2	PO4	C	505	-	4,4,4	1.16	0	6,6,6	0.27	0
2	PO4	C	507	-	4,4,4	1.10	0	6,6,6	0.27	0
2	PO4	C	511	-	4,4,4	1.16	0	6,6,6	0.27	0
2	PO4	D	506	-	4,4,4	1.04	0	6,6,6	0.27	0
2	PO4	D	508	-	4,4,4	1.13	0	6,6,6	0.27	0
2	PO4	D	512	-	4,4,4	1.04	0	6,6,6	0.27	0
2	PO4	E	504	-	4,4,4	0.91	0	6,6,6	0.27	0
2	PO4	E	509	-	4,4,4	1.04	0	6,6,6	0.27	0
2	PO4	F	502	-	4,4,4	1.09	0	6,6,6	0.27	0
2	PO4	F	510	-	4,4,4	1.07	0	6,6,6	0.27	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
2	PO4	A	501	-	-	0/0/0/0	0/0/0/0
2	PO4	B	503	-	-	0/0/0/0	0/0/0/0
2	PO4	C	505	-	-	0/0/0/0	0/0/0/0
2	PO4	C	507	-	-	0/0/0/0	0/0/0/0
2	PO4	C	511	-	-	0/0/0/0	0/0/0/0
2	PO4	D	506	-	-	0/0/0/0	0/0/0/0
2	PO4	D	508	-	-	0/0/0/0	0/0/0/0
2	PO4	D	512	-	-	0/0/0/0	0/0/0/0
2	PO4	E	504	-	-	0/0/0/0	0/0/0/0
2	PO4	E	509	-	-	0/0/0/0	0/0/0/0
2	PO4	F	502	-	-	0/0/0/0	0/0/0/0
2	PO4	F	510	-	-	0/0/0/0	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	507	PO4	1	0
2	D	512	PO4	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

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

### 6.4 Ligands [i](#)

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

### 6.5 Other polymers [i](#)

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